KOH II → I

Enter NEWS followed by the item number or name to see news on that
specific topic.

* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:29:37 ON 15 DEC 2006

=> file casreact
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

FILE 'CASREACT' ENTERED AT 12:29:52 ON 15 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 11 Dec 2006 VOL 145 ISS 24

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*   *
*   CASREACT now has more than 10 million reactions   *
*   *
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10522622\1.KOH+II-I.str
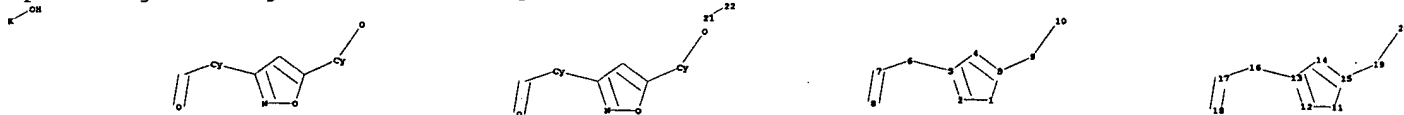
chain nodes :
6 7 8 9 10 16 17 18 19 20 21 22
ring nodes :
1 2 3 4 5 11 12 13 14 15
chain bonds :
3-6 5-9 6-7 7-8 9-10 13-16 15-19 16-17 17-18 19-20 21-22
ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15
exact/norm bonds :
1-2 1-5 2-3 3-4 3-6 4-5 5-9 6-7 7-8 9-10 11-12 11-15 12-13 13-14 13-16
14-15 15-19 16-17 17-18 19-20
exact bonds :
21-22

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom
20:CLASS 21:CLASS 22:CLASS
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
containing 21

L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 12:30:13 FILE 'CASREACT'
SCREENING COMPLETE -   6077 REACTIONS TO VERIFY FROM   455 DOCUMENTS

100.0% DONE   6077 VERIFIED   3 HIT RXNS   2 DOCS
SEARCH TIME: 00.00.02
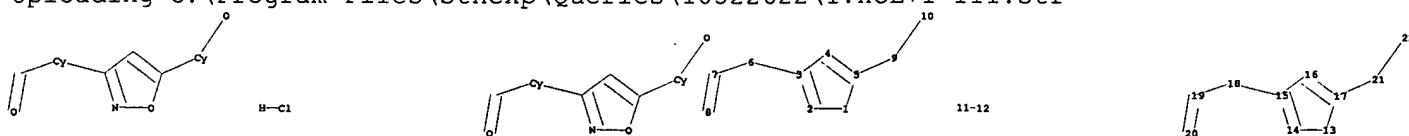
L2   2 SEA SSS FUL L1 (3 REACTIONS)

=> d ibib hit 1-2

I   HCl   →   III

```
=>
Uploading C:\Program Files\Stnexp\Queries\10522622\1.HCL+I-III.str
```



```
chain nodes :
6  7  8  9  10  11  12  18  19  20  21  22
ring nodes :
1  2  3  4  5  13 ·14  15  16  17
chain bonds :
3-6  5-9  6-7  7-8  9-10  11-12  15-18  17-21  18-19  19-20  21-22
ring bonds :
1-2  1-5  2-3  3-4  4-5  13-14  13-17  14-15  15-16  16-17
exact/norm bonds :
1-2  1-5  2-3  3-4  3-6  4-5  5-9  6-7  7-8  9-10  13-14  13-17  14-15  15-16  15-18
16-17  17-21  18-19  19-20  21-22
exact bonds : .
11-12


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:CLASS
20:CLASS  21:Atom  22:CLASS
fragments assigned product role:
containing 13
fragments assigned reactant/reagent role:
containing 1
containing 11




L3        STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3                STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l3 full
FULL SEARCH INITIATED 12:31:00 FILE 'CASREACT'
SCREENING COMPLETE -    23962 REACTIONS TO VERIFY FROM      1991 DOCUMENTS

100.0% DONE   23962 VERIFIED       5 HIT RXNS                      2 DOCS
SEARCH TIME: 00.00.04

L4              2 SEA SSS FUL L3 (      5 REACTIONS)

=> d ibib hit 1-2
```
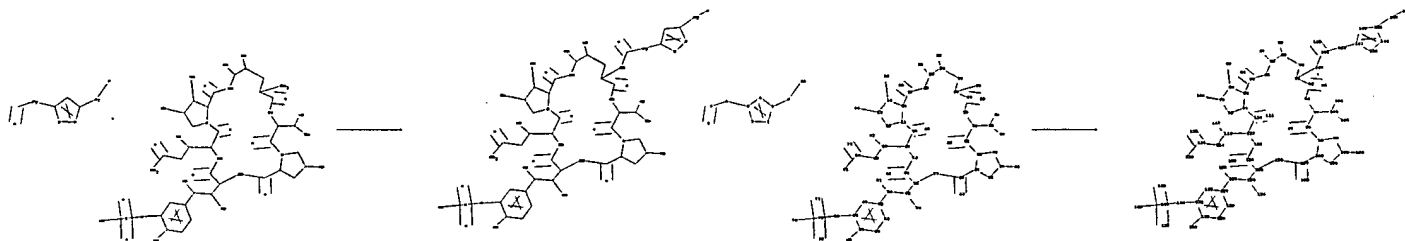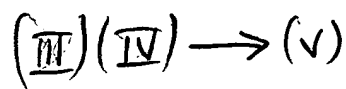
$$(\underline{\text{III}})(\underline{\text{IV}}) \longrightarrow (\text{V})$$

chain nodes :
6   7   8   9   10   16   18   21   22   26   28   32   38   39   40   41   43   44   46   48   49   50   51
52   55   58   59   60   61   68   69   70   71   72   73   74   82   84   87   88   93   97   103   104   105
106   108   109   111   113   114   115   116   117   120   123   124   125   126   133   134   135   136
137   138   139   140   141   142   143   149   150
ring nodes :
1   2   3   4   5   11   12   13   14   15   17   19   20   23   24   25   27   29   30   31   33   34   35   36
37   42   45   47   53   54   56   57   62   63   64   65   66   67   77   78   79   80   81   83   85   86
89   90   91   92   94   95   96   98   99   100   101   102   107   110   112   118   119   121   122   127
128   129   130   131   132   144   145   146   147   148
chain bonds :
3-6   5-9   6-7   7-8   9-10   13-44   14-16   17-18   20-21   22-23   25-26   27-28   30-38   31-32
35-41   38-39   38-40   42-43   45-46   47-48   48-49   48-52   49-50   50-51   50-73   54-55   56-58
58-59   58-60   60-61   60-62   65-68   66-69   69-70   70-71   70-72   70-74   79-109   80-82
83-84   86-87   88-89   91-140   92-93   95-103   96-97   100-106   103-104   103-105   107-108
110-111   112-113   113-114   113-117   114-115   115-116   115-138   119-120   121-123   123-124
123-125   125-126   125-127   130-133   131-134   134-135   135-136   135-137   135-139   140-141
141-142   141-143   143-147   145-149   149-150
ring bonds :
1-2   1-5   2-3   3-4   4-5   11-12   11-15   11-45   12-13   13-14   14-15   15-17   17-19   19-20
20-23   23-24   24-25   25-27   27-29   29-30   30-31   31-33   33-34   33-37   34-35   35-36   36-37
37-42   42-57   45-47   47-53   53-54   54-56   56-57   62-63   62-67   63-64   64-65   65-66
66-67   77-78   77-81   77-110.   78-79   79-80   80-81   81-83   83-85   85-86   86-89   89-90
90-91   91-92   92-94   94-95   95-96   96-98   98-99   98-102   99-100   100-101   101-102
102-107   107-122   110-112   112-118   118-119   119-121   121-122   127-128   127-132   128-129
129-130   130-131   131-132   144-148   144-145   145-146   146-147   147-148
exact/norm bonds :
1-2   1-5   2-3   3-4   3-6   4-5   5-9   6-7   7-8   9-10   11-12   11-15   11-45   12-13   13-14
14-15   14-16   15-17   17-18   17-19   19-20   20-21   20-23   22-23   23-24   24-25   25-26   25-27
27-28   27-29   29-30   30-31   31-32   31-33   33-34   33-37   34-35   35-36   35-41   36-37
37-42   38-39   42-43   42-57   45-46   45-47   47-53   48-52   50-51   50-73   53-54   54-55   54-56
56-57   58-59   60-61   65-68   66-69   69-70   77-78   77-81   77-110   78-79   79-80   80-81
80-82   81-83   83-84   83-85   85-86   86-87   86-89   88-89   89-90   90-91   91-92   91-140
92-93   92-94   94-95   95-96   96-97   96-98   98-99   98-102   99-100   100-101   100-106
101-102   102-107   103-104   107-108   107-122   110-111   110-112   112-118   113-117   115-116
115-138   118-119   119-120   119-121   121-122   123-124   125-126   130-133   131-134   134-135
140-141   141-142   141-143   143-147   144-148   144-145   145-146   145-149   146-147   147-148
149-150
exact bonds :
13-44   30-38   38-40   47-48   48-49   49-50   56-58   58-60   60-62   79-109   95-103   103-105
112-113   113-114   114-115   121-123   123-125   125-127
normalized bonds :
62-63   62-67   63-64   64-65   65-66   66-67   70-71   70-72   70-74   127-128   127-132   128-129
129-130   130-131   131-132   135-136   135-137   135-139

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:CLASS 19:Atom
20:Atom 21:CLASS 22:CLASS 23:Atom 24:Atom 25:Atom 26:CLASS 27:Atom 28:CLASS
29:Atom 30:Atom 31:Atom 32:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom
38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:CLASS 44:CLASS 45:Atom 46:CLASS
47:Atom 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:Atom 54:Atom 55:CLASS
56:Atom 57:Atom 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:Atom 63:Atom 64:Atom
65:Atom 66:Atom 67:Atom 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS
74:CLASS 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:CLASS 83:Atom 84:CLASS
85:Atom 86:Atom 87:CLASS 88:CLASS 89:Atom 90:Atom 91:Atom 92:Atom 93:CLASS
94:Atom 95:Atom 96:Atom 97:CLASS 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom
103:CLASS 104:CLASS 105:CLASS 106:CLASS 107:Atom 108:CLASS 109:CLASS 110:Atom
111:CLASS 112:Atom 113:CLASS 114:CLASS 115:CLASS 116:CLASS 117:CLASS 118:Atom
119:Atom 120:CLASS 121:Atom 122:Atom 123:CLASS 124:CLASS 125:CLASS 126:CLASS
127:Atom 128:Atom 129:Atom 130:Atom 131:Atom 132:Atom 133:CLASS 134:CLASS
135:CLASS 136:CLASS 137:CLASS 138:CLASS 139:CLASS 140:CLASS 141:CLASS 142:CLASS
143:Atom 144:Atom 145:Atom 146:Atom 147:Atom 148:Atom 149:Atom 150:CLASS
fragments assigned product role:
containing 77
fragments assigned reactant/reagent role:
containing 1
containing 11

L5   STRUCTURE UPLOADED

=> s l5 full
FULL SEARCH INITIATED 12:46:32 FILE 'CASREACT'
SCREENING COMPLETE -   2 REACTIONS TO VERIFY FROM   1 DOCUMENTS

100.0% DONE   2 VERIFIED   2 HIT RXNS   1 DOCS
SEARCH TIME: 00.00.01

L6   1 SEA SSS FUL L5 (2 REACTIONS)

=> d ibib hit 1

10/522,622 12/15/2006

```
=> file reg
COST IN U.S. DOLLARS                    SINCE FILE      TOTAL
                                          ENTRY        SESSION
FULL ESTIMATED COST                     118.68         361.01
```

FILE 'REGISTRY' ENTERED AT 12:51:24 ON 15 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 14 DEC 2006   HIGHEST RN 915690-78-7
DICTIONARY FILE UPDATES: 14 DEC 2006   HIGHEST RN 915690-78-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

    Please note that search-term pricing does apply when
    conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

```
=>
Uploading C:\Program Files\Stnexp\Queries\10522622\17.str
```
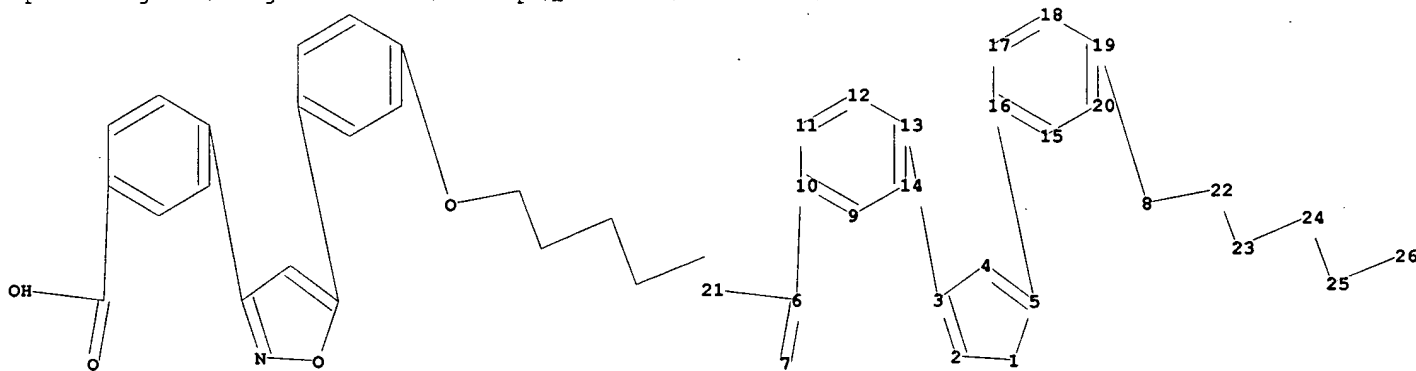


```
chain nodes :
6  7  8  21  22  23  24  25  26
ring nodes :
1  2  3  4  5  9  10  11  12  13  14  15  16  17  18  19  20
chain bonds :
3-13  5-16  6-7  6-10  6-21  8-19  8-22  22-23  23-24  24-25  25-26
ring bonds :
1-2  1-5  2-3  3-4  4-5  9-10  9-14  10-11  11-12  12-13  13-14  15-16  15-20  16-17
17-18  18-19  19-20
exact/norm bonds :
1-2  1-5  2-3  3-4  4-5  8-19  8-22
```

10/522,622 12/15/2006

exact bonds :
3-13 5-16 6-10 22-23 23-24 24-25 25-26
normalized bonds :
6-7 6-21 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17 17-18 18-19
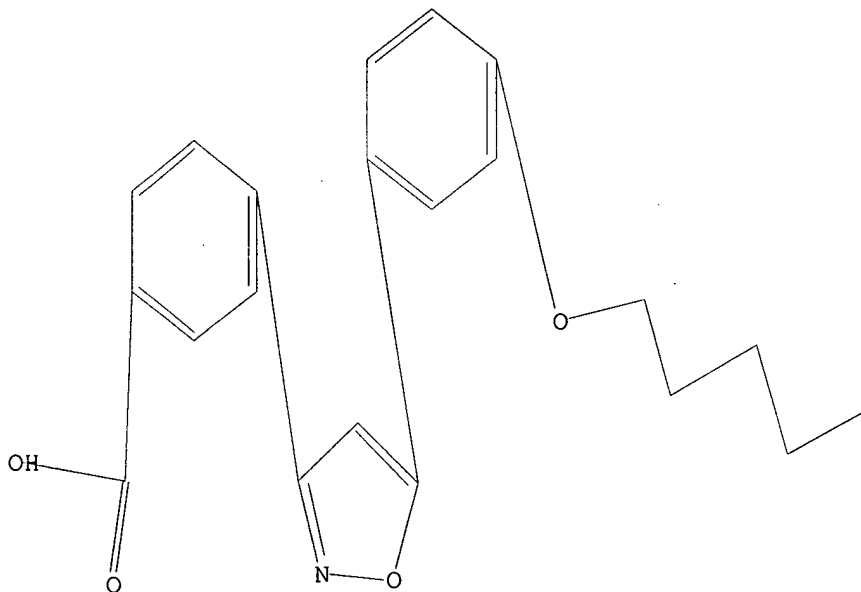19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L7   STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7   STR

Structure attributes must be viewed using STN Express query preparation.

=> s l7 full
FULL SEARCH INITIATED 12:51:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   402 TO ITERATE

100.0% PROCESSED   402 ITERATIONS   7 ANSWERS
SEARCH TIME: 00.00.01

L8   7 SEA SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                              ENTRY   SESSION
FULL ESTIMATED COST   166.94   527.95

FILE 'CAPLUS' ENTERED AT 12:51:43 ON 15 DEC 2006

FILE COVERS 1907 - 15 Dec 2006   VOL 145 ISS 26
FILE LAST UPDATED: 14 Dec 2006   (20061214/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
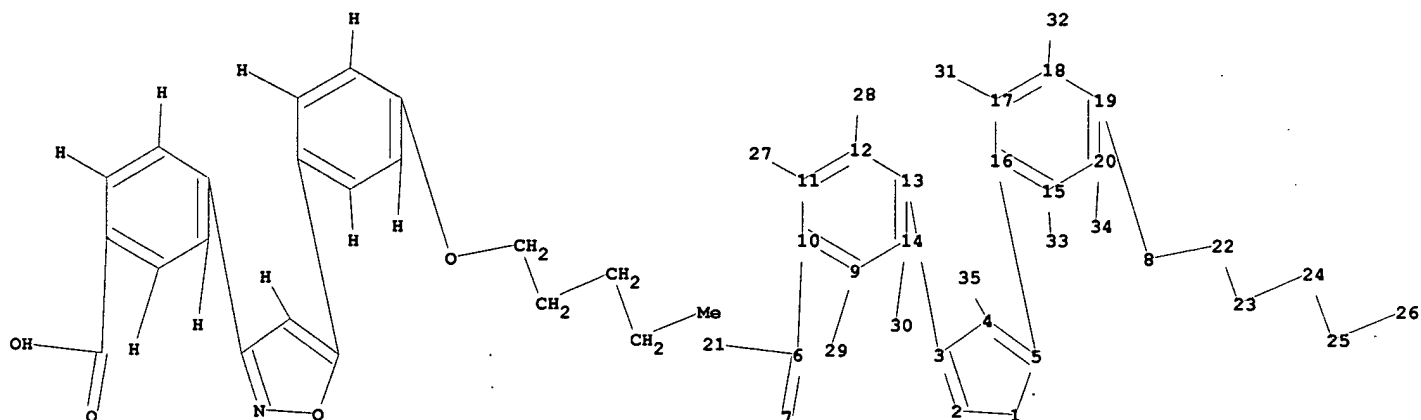They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l8
L9   5 L8

=> d ibib hitstr 1-5

chain nodes :
6 7 8 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35
ring nodes :
1 2 3 4 5 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
3-13 4-35 5-16 6-7 6-10 6-21 8-19 8-22 9-29 11-27 12-28 14-30 15-33 17-31
18-32 20-34 22-23 23-24 24-25 25-26
ring bonds :
1-2 1-5 2-3 3-4 4-5 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17
17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 8-19
exact bonds :
3-13 4-35 5-16 6-10 8-22 9-29 11-27 12-28 14-30 15-33 17-31 18-32 20-34
22-23 23-24 24-25 25-26
normalized bonds :
6-7 6-21 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17 17-18 18-19
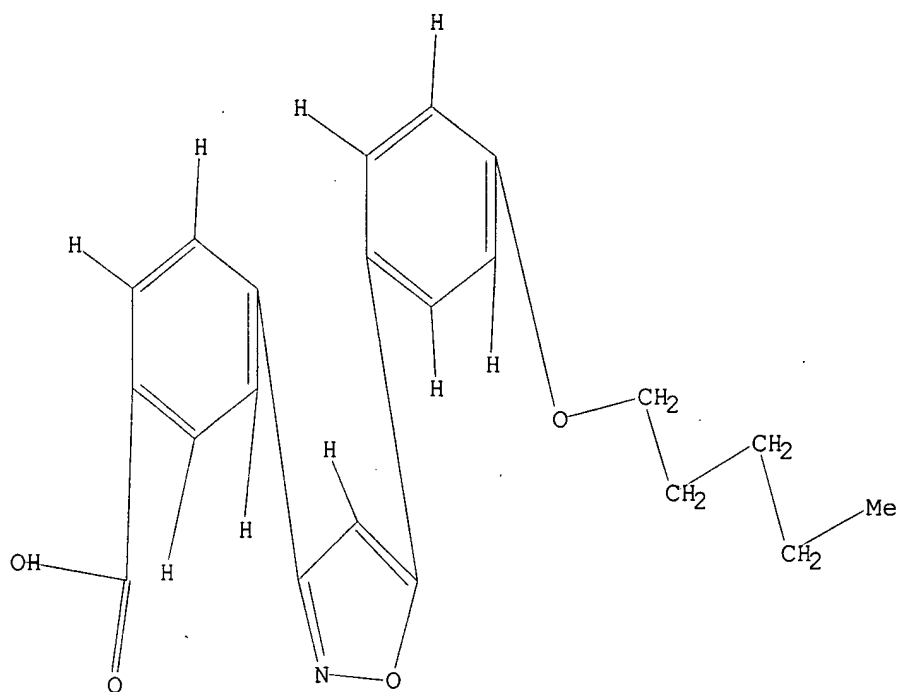19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS

L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR

Structure attributes must be viewed using STN Express query preparation.


```
=> s l1 full
FULL SEARCH INITIATED 13:02:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      402 TO ITERATE

100.0% PROCESSED      402 ITERATIONS                          3 ANSWERS
SEARCH TIME: 00.00.01

L2             3 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                      SINCE FILE      TOTAL
                                            ENTRY        SESSION
FULL ESTIMATED COST                        166.94        167.15
```

FILE 'CAPLUS' ENTERED AT 13:03:03 ON 15 DEC 2006
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FILE COVERS 1907 - 15 Dec 2006   VOL 145 ISS 26
FILE LAST UPDATED: 14 Dec 2006   (20061214/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2
L3   3 L2

=> d ibib hitstr 1-3